



There is now broad agreement among scientists, scientific societies, and government agencies that growing atmospheric CO₂ concentrations resulting from the burning of fossil fuels are causing increases in global atmospheric temperature. These temperature increases are projected to disrupt climate, warm the oceans, and melt continental ice sheets, leading to sea level rise. Avoiding the widespread and potentially disastrous consequences of climate change and sea-level rise depends on the ability of mankind to rapidly reduce CO₂ emissions.

Experts believe that to avoid significant disruption of the climate system and ecosystems, CO₂ concentrations must be stabilized within the next several decades. At today's emission rates of approximately 30 Gt CO₂/year from the burning of fossil fuels, CO₂ concentrations will continue to grow and, within 50 years, may exceed the levels needed to protect sensitive agricultural and ecosystems and avoid flooding in low-lying coastal areas. This situation is even more urgent when we consider that, over the next 50 years, CO₂ emissions are expected to double as the developing world's economies grow and the global standard of living increases.

Research Program GEOLOGIC CARBON SEQUESTRATION PROGRAM

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One strategy to reduce effective CO₂ emissions that has quickly advanced from a mere concept to a reality is the geologic storage of CO₂ in underground formations. Significant progress has been made in the critical areas of geologic storage security and integrity, storage optimization, monitoring and verification, and risk assessment and mitigation. While additional research and testing remain to be accomplished before the technology can be applied widely, results of research conducted in various projects at Berkeley Lab and elsewhere demonstrate that this technology can make large contributions to the problem of reducing point-source CO₂ emissions for climate-change mitigation.

On April 7, 2007, following nearly ten years of pioneering involvement in geologic carbon sequestration, the Earth Sciences Division added a new program, the Geologic Carbon Sequestration (GCS) Program. The GCS program is dedicated to addressing the pressing need for drastic reductions in CO₂ emissions, while recognizing that fossil fuels will continue to be used for decades if not centuries. The GCS currently includes four main projects:

- GeoSeq
- West Coast Regional Carbon Sequestration Partnership (WESTCARB)
- Zero Emissions Research and Technology (ZERT)
- CO₂ Geological Storage and Groundwater Resources

Each of these projects is focused on specific aspects of GCS. For example, GeoSeq focuses on scientific field testing and analysis of geologic storage including projects overseas. WESTCARB is a partnership for the purpose of pilot testing in western North America to demonstrate the potential for CO₂ storage in deep geological formations and to enable deployment of CCS technology. ZERT performs fundamental research on geologic storage. The potential impact of large-scale geologic sequestration of CO₂ on groundwater quality and hydrology is investigated in the fourth project.

GEOSEQ

The GeoSeq Project has two primary goals:

- (1) To develop ways to improve predictions of injectivity and effective capacity of saline formations and depleted gas reservoirs, and
- (2) To develop and test innovative high-resolution methods for monitoring CO₂ in the subsurface.

The GeoSeq project leverages scientific understanding and technology development from three highly visible, ongoing world-class (Carbon Sequestration Leadership Forum (CSLF)-recognized) geologic CO₂ storage projects, through leadership and collaboration in the scientific and engineering objectives. The three projects are the:

- (1) Frio Brine Pilot Tests
- (2) Otway Basin Pilot Project
- (3) In Salah Industrial-Scale CO₂ Storage Project

Within these projects, GeoSeq has led the development of downhole fluid and gas sampling by U-tube, downhole continuous active source seismic monitoring (CASSM), and reservoir simulation capabilities, including reactive geochemistry, multi-component gas mixtures, and geomechanical coupling.

We continue to advance understanding of CO₂ migration in brine formations and depleted gas reservoirs, and to investigate the geomechanical effects of industrial-scale CO₂ injection. Although the three projects are carried out in distinct geological environments, the scope of GeoSeq is integrative, with strong cross-task communication and application of common tools and approaches in related projects. The overall objective of the GeoSeq project is to gain knowledge of geologic CO₂ storage processes and mechanisms, and how to monitor and simulate them while making results available through publications and conference participation. Advances derived from GeoSeq efforts also support the DOE Regional Partnership Projects through the involvement of the investigators in various Partnership projects, and will likely be used in commercial-scale CO₂ operations in the future.

WESTCARB

The West Coast Regional Carbon Sequestration Partnership (WESTCARB) is a public-private partnership aimed at assessing carbon sequestration opportunities in the Western United States and Canada. The effort is led by the California Energy

Commission, which is responsible for the overall conduct of the work. The effort involves numerous private sector and public sector partners, who will be responsible for carrying out various aspects of the project. Overarching goals of the WESTCARB Phase III effort recently announced include:

- (1) Promoting a better understanding of injectivity, capacity, and storativity of CO₂ in typical West Coast formations
- (2) Demonstrating the security and commercial viability of industrial-scale CO₂ storage in a deep saline formation to pave the way for future widespread West Coast deployment of CO₂ capture and geologic storage.

Lawrence Berkeley National Laboratory's contribution to the proposed work for the WESTCARB Phase III effort will cover the following:

- (1) Site characterization efforts in support of local and regional reservoir model development, evaluation of formation capacity and injectivity, and regulatory permitting
- (2) Risk assessment and mitigation planning in support of site selection, public safety, environmental protection, storage effectiveness, and regulatory permitting
- (3) Performance monitoring in support of public safety, environmental protection, regulatory oversight, and demonstration of storage effectiveness.

ZERT

Carbon dioxide capture and storage in deep geologic formations has quickly emerged as one of the most promising options for reducing carbon dioxide emissions from combustion of fossil fuels. Potential storage formations include depleted oil and gas reservoirs, deep salt-water filled formations (saline formations), and unminable coal beds. ZERT focuses on developing fundamental knowledge needed to ensure successful storage in saline formations and hydrocarbon reservoirs. Topics of this study include the following:

- (1) Performance prediction for underground fate and transport of CO₂
- (2) Measurement and monitoring techniques to verify storage and track migration of CO₂
- (3) Fundamental geochemical and hydrological investigations of CO₂ storage



The approach will include a combination of theoretical investigations, field studies, computer simulation, and laboratory experiments. Where appropriate, the applicability of these results to other types of storage formations will be identified.

CO₂ GEOLOGIC STORAGE & GROUNDWATER RESOURCES (EPA-NETL)

This project addresses concerns about the nation's groundwater resources and the potential impacts of large-scale deployment of geologic carbon sequestration on groundwater. For example, leakage of CO₂ from depth and subsequent migration into shallow aquifers could result in water quality changes. Furthermore, the displacement of native brines caused by injection of large volumes of CO₂ could impact the basin-scale hydrology of shallower groundwater systems, depending on the level of hydraulic communication between them. Two primary research tasks address these concerns, jointly coordinated by the U.S. Environmental Protection Agency (EPA) and the National Energy Technology Laboratory (NETL):

1. Understanding groundwater quality changes in case of CO₂ intrusion (Task A)
2. Large-scale hydrological evaluation and modeling of impact on groundwater systems (Task B)

Both tasks are currently in the first year of a three-year research effort.

FUNDING

The GCS Program receives the bulk of its funding both directly and indirectly (e.g., indirectly through collaboration with regional partnership groups) from the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, National Energy Technology Laboratory, of the U.S. Department of Energy under U.S. Department of Energy Contract No. DE-AC02-05CH11231. Additional support is provided by the U.S. Environmental Protection Agency (EPA), the Carbon Capture Project (CCP), and various other sources through the Berkeley Lab Work for Others program.



LARGE-SCALE HYDROLOGICAL EVALUATION OF CO₂ INJECTION-STORAGE AND MODELING OF THE IMPACT ON GROUNDWATER SYSTEMS

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RESEARCH OBJECTIVES

If carbon dioxide capture and storage (CCS) technologies are implemented, the amount of CO₂ injected and sequestered underground will be extremely large. To date, the impact of large-scale injection and related brine displacement on regional multilayered groundwater systems has not been systematically assessed. The present project aims at enhancing understanding of the increase and extent of water pressure in the storage formation and in the shallower aquifers, due to injection of large amounts of supercritical CO₂. In particular, the change in groundwater table level, the effect on discharge and recharge zones in the groundwater system, and the impact of these changes on the properties and characteristics of underground sources of drinking water (USDWs) will be investigated systematically.

APPROACH

A series of studies is being conducted with successive degrees of complexity, leading up to detailed modeling of one or two selected basin-scale groundwater systems in the United States with potential for large-scale CO₂ sequestration. The first study is a systematic evaluation of storage capacity and pressure buildup in compartmentalized storage formations, where the native brine cannot easily escape because of closed boundaries. The second study assumes open multilayered groundwater systems and evaluates the potential impacts of brine displacement on shallow aquifers. Impact of coupled hydromechanical effects will be evaluated in the third study. Finally, the fourth study is an analysis and modeling of one or two representative basin-scale groundwater systems.

ACCOMPLISHMENTS

Results from a multiphase simulation model for CO₂ injection into a compartmentalized saline formation were obtained as a function of storage formation volume and hydrogeologic characteristics. An example is shown in Figure 1. Based on comparison with simulation results, simple quick-assessment methods were developed for estimating the storage capacity in such pressure-constrained systems. We have also started a simulation study investigating CO₂ injection into a multilayer system with open lateral boundaries as a function of the permeability of the upper and lower sealing units. It was found that the presence of low-permeability sealing layers may significantly affect

fluid-pressure buildup and brine displacement for both laterally open and closed systems.

SIGNIFICANCE OF FINDINGS

Simple, quick-assessment methods for estimating storage capacity in pressure-constrained systems may prove to be valuable in practical applications, such as selection of an optimal site among several possibilities. The indicated significant influence of vertical brine movements through upper and lower confining layers on storage capacity may have been ignored in many large-scale studies to date. These will be further investigated. Papers summarizing results of the present research are being prepared for submission to journals.

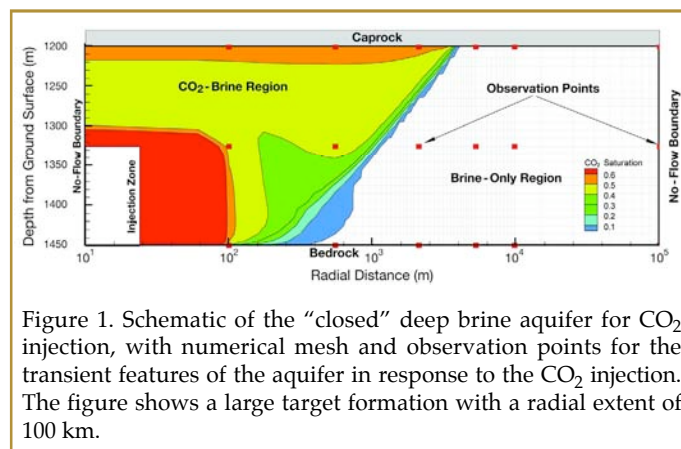


Figure 1. Schematic of the “closed” deep brine aquifer for CO₂ injection, with numerical mesh and observation points for the transient features of the aquifer in response to the CO₂ injection. The figure shows a large target formation with a radial extent of 100 km.

RELATED PUBLICATION

Zhou, Q., J. Birkholzer, J. Rutqvist, and C.-F. Tsang, Sensitivity study of CO₂ capacity in brine aquifers with closed boundaries: Dependence on hydrogeologic properties. Abstract Submitted to 6th Annual Conference on Carbon Capture and Sequestration, Pittsburgh, PA, May 2007.

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal and Power Systems, through the National Energy Technologies Laboratory (NETL), under the auspices of U.S. Department of Energy Contract No. DE-AC02-05CH11231.

GEOCHEMICAL INVESTIGATIONS OF THE VULNERABILITY OF GROUNDWATER RESOURCES IN CASE OF CO₂ LEAKAGE FROM DEEP GEOLOGIC STORAGE

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RESEARCH OBJECTIVES

If carbon dioxide stored in deep saline aquifers leaks into overlying sources of potable groundwater, the intruding CO₂ would lower groundwater pH and thereby enhance the solubility of hazardous inorganic constituents (e.g., lead and arsenic). How and to what extent groundwater potability would be affected depend largely on the initial abundance and distribution of these constituents in the aquifers, as well as on the aquifer mineralogy and the oxidation state. The research objective is to understand in a general sense (1) which aquifer systems and regions of the United States might be vulnerable in case of CO₂ intrusion, and (2) which inorganic constituents might adversely affect water quality and to what extent.

APPROACH

A database analysis is being conducted to evaluate almost 40,000 groundwater samples taken throughout the United States that report non-zero concentrations of selected hazardous constituents. Equilibrium models of aquifer chemistry are being developed to estimate the initial distribution of these hazardous constituents between the aqueous phase and adsorption and ion exchange sites, and in solid solution in primary and secondary minerals. The equilibrium models are then used as a starting point to (1) simulate the redistribution of hazardous constituents between the host rock and the groundwater in the case of CO₂ intrusion with reactive transport models and (2) to predict the expected aqueous concentrations of such constituents for a range of relevant aquifer conditions. Laboratory experiments will also be conducted to validate and support the numerical results.

ACCOMPLISHMENTS

Data from almost 40,000 groundwater samples have been systematically evaluated in an automated procedure involving data management systems and distribution-of-species modeling. Results provide valuable information on the relevant geochemical conditions in aquifers defining the vulnerability of aquifers in case of CO₂ intrusion. For example, we identified the fraction of groundwaters where minerals control the activity of hazardous constituents in the aqueous phase (which makes them vulnerable) and determined the number of samples that are saturated with respect to calcite (which makes them less vulnerable—Figure 1). In parallel to the database evaluation, a large number of reactive transport simulations have been conducted for modeling the mobilization of lead and arsenic in response to the intrusion of gaseous CO₂ into a shallow aquifer. Various sensitivities have been evaluated related to aquifer conditions (e.g., CO₂ intrusion rate, aquifer hydrogeology), geochemical parameters (e.g., rock mineralogy, thermodynamic data) and processes (e.g., adsorption/desorption, cation exchange, co-precipitation).

SIGNIFICANCE OF FINDINGS

Our preliminary results demonstrate that CO₂-related dissolution may strongly increase concentrations of lead and arsenic in the groundwater, indicating the significance of this subject for geologic carbon sequestration. However, the simulations conducted to date arrive at water contamination above health-based limits only when very conservative assumptions are made with respect to the aquifer geochemical conditions. Our ongoing study will use more realistic scenarios and will be supplemented by laboratory experiments. Once completed, this research will provide a systematic evaluation of main aquifer types and determine their vulnerability in case of CO₂ intrusion.

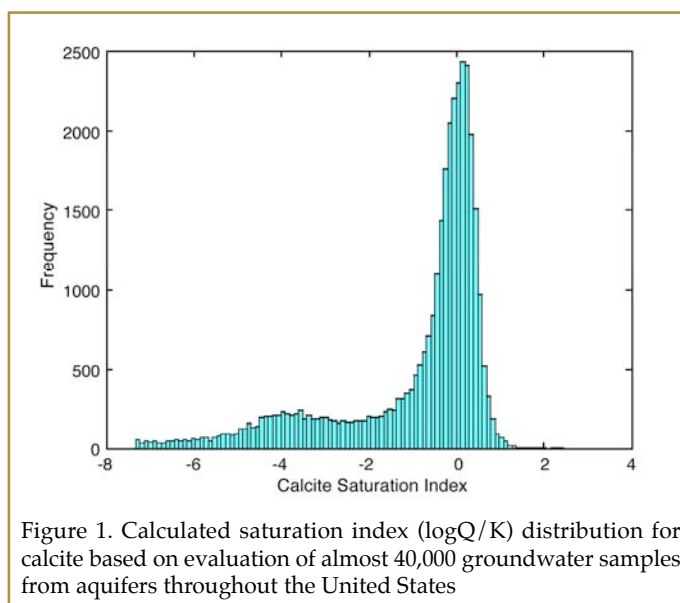


Figure 1. Calculated saturation index (logQ/K) distribution for calcite based on evaluation of almost 40,000 groundwater samples from aquifers throughout the United States

RELATED PUBLICATIONS

Xu, T., J. Apps, and J. Birkholzer, Contamination of groundwater by hazardous inorganic chemical constituents through induced acidification due to CO₂ leakage from a storage formation. Abstract in Proceedings of the 6th Annual Conference on Carbon Capture and Sequestration, Pittsburgh, PA, May 2007.

Zhang, Y., J.A. Apps, J.A. Birkholzer, T. Xu, and C.-F. Tsang, A database analysis of the distribution of hazardous metals in groundwaters of the United States. Abstract in Proceedings 6th Annual Conference on Carbon Capture and Sequestration, Pittsburgh, PA, May 2007.

ACKNOWLEDGMENTS

This work was supported by the U.S. Environmental Protection Agency, Office of Water and Office of Air and Radiation, under an Interagency Agreement with the U.S. Department of Energy and Lawrence Berkeley National Laboratory.



OPTIMALITY IN CHARACTERIZING CO₂ SEEPAGE FROM GEOLOGIC CARBON SEQUESTRATION SITES

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RESEARCH OBJECTIVES

Surface monitoring to ensure safe and effective CO₂ storage is complicated by the large area that may need to be monitored, and by large fluctuations in natural background CO₂ fluxes and concentrations. These complications make seepage (surface CO₂ leakage) monitoring potentially very expensive. We adopt the philosophy that *monitoring* is the activity involved in detecting and locating seepage areas, while *measurements* are made to pinpoint and quantify seepage once it is detected. To be effective at detecting seepage, a monitoring program must be affordable enough to carry out and therefore requires optimization. In this work, we explore various optimization strategies for characterizing seepage using near-surface measurement approaches such as accumulation chambers and eddy covariance towers.

APPROACH

We are using a combination of theoretical and numerical approaches. Simulations of CO₂ seepage in a 3-D system with variable topography were carried out using TOUGH2/EOS7CA to generate a virtual seepage signal. The resulting virtual CO₂ concentrations were analyzed using MATLAB routines for artificial neural networks (ANNs) and particle swarm optimization (PSO) to develop a promising approach for optimizing seepage characterization.

ACCOMPLISHMENTS

Assuming no a priori knowledge of where seepage will occur, a static grid-based arrangement of monitoring stations (e.g., eddy covariance towers) is the only configuration suitable to ensure detection of seepage above some threshold value. The fixed-grid approaches needed to detect seepage are expected to require large numbers of eddy covariance towers for large-scale geologic CO₂ storage. Once seepage has been detected and roughly located using a fixed grid approach, seepage zones and features can be optimally pinpointed through a dynamic search strategy, e.g., employing accumulation chambers and/or soil-gas sampling. Quantification of seepage rates can be done through measurements on a localized fixed grid once the seepage is pinpointed.

ANNs can be used as regression models for distinguishing natural system behavior from CO₂ seepage without the need for detailed

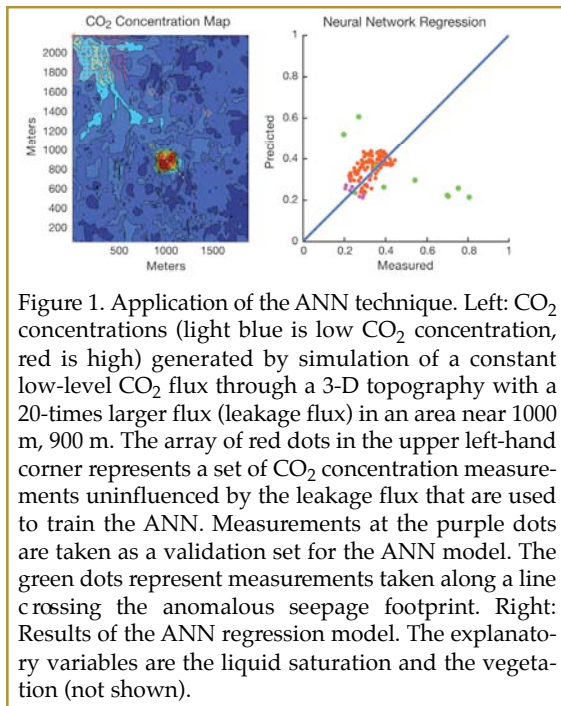


Figure 1. Application of the ANN technique. Left: CO₂ concentrations (light blue is low CO₂ concentration, red is high) generated by simulation of a constant low-level CO₂ flux through a 3-D topography with a 20-times larger flux (leakage flux) in an area near 1000 m, 900 m. The array of red dots in the upper left-hand corner represents a set of CO₂ concentration measurements uninfluenced by the leakage flux that are used to train the ANN. Measurements at the purple dots are taken as a validation set for the ANN model. The green dots represent measurements taken along a line crossing the anomalous seepage footprint. Right: Results of the ANN regression model. The explanatory variables are the liquid saturation and the vegetation (not shown).

understanding of natural system processes. An example of the use of ANNs for seepage detection is shown in Figure 1. Because of natural variability, simple steepest-descent algorithms are not effective, and evolutionary computation algorithms are proposed as a paradigm for dynamic monitoring networks to pinpoint CO₂ seepage areas. One such approach is PSO, in which a swarm of particles is assigned a random position and velocity to sample the search space. We used PSO to locate the CO₂ seepage anomaly in the virtual landscape of Figure 1. Convergence to the global minimum was achieved in the majority of the runs for different random initializations. Additional analyses will need to be undertaken for a better understanding of convergence and convergence rates.

SIGNIFICANCE OF FINDINGS

The expense anticipated to carry out effective geologic CO₂ storage monitoring motivates optimization. We find that ANNs and PSO are promising approaches for lowering the cost of CO₂ seepage characterization.

RELATED PUBLICATIONS

Cortis, A., C.M. Oldenburg, and S.M. Benson, On the optimality of above-ground monitoring networks for carbon capture and storage. LBNL-62512 Abs. Sixth Annual Conference on Carbon Capture and Sequestration, Pittsburgh, PA, May 8-10, 2007, Oldenburg, C.M., A. Cortis, and S.M. Benson, Near-Surface Dispersion of CO₂ Seepage from Geologic Storage Sites: Interplay of Process and Detection Strategy. LBNL-62875 Abs. American Geophys. Union Fall Meeting, San Francisco, CA, Dec. 2006.

ACKNOWLEDGMENTS

This work was conducted as part of the Zero Emissions Research and Technology (ZERT) project, supported by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, through the National Energy Technology Laboratory, U.S. Department of Energy, under Contract No. DE-AC02-05CH11231. Hydrogen and Clean Coal Fuels, through the National Energy Technology Laboratory, U.S. Department of Energy, under Contract No. DE-AC02-05CH11231.



CONTINUOUS ACTIVE-SOURCE SEISMIC MONITORING (CASSM) FOR CO₂ INJECTION IN A BRINE AQUIFER

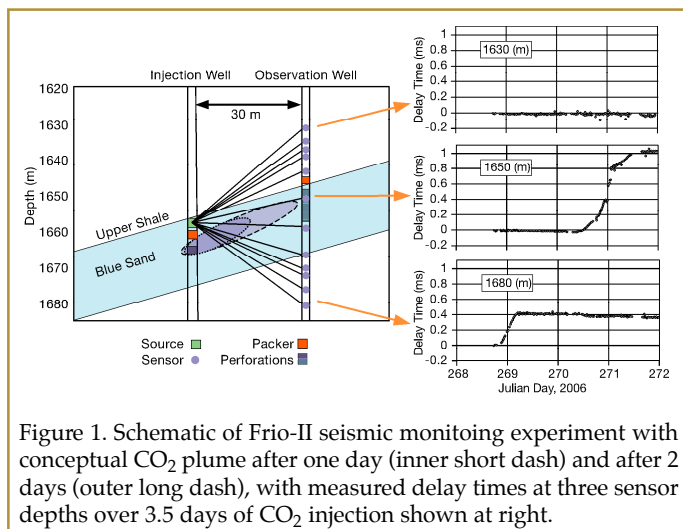
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RESEARCH OBJECTIVES

Monitoring of subsurface CO₂ storage is a key component of carbon sequestration. As part of a small-scale CO₂ injection, known as the Frio-II experiment, we developed a novel crosswell seismic monitoring approach, which would allow continuous crosswell monitoring during injection through use of a borehole source deployed in the injection well. The Frio-II experiment had the goal of monitoring CO₂ plume migration under conditions strongly affected by buoyancy of CO₂ in the brine aquifer. Monitoring buoyancy required crosswell geophysical measurements because fluid sampling in the observation well could not be relied on to detect the depth of initial CO₂ breakthrough within the reservoir interval.



APPROACH

Time-lapse crosswell tomographic imaging of the Frio-I CO₂ plume demonstrated that large changes in seismic velocity (a 500 m/s decrease within the plume) were caused by the injection of supercritical CO₂ into the brine reservoir. The large seismic velocity change measured in the Frio-I test suggested that continuous monitoring of crosswell travel time during injection could detect CO₂ saturation changes along a given raypath. Therefore, we designed a crosswell CASSM experiment for Frio-II in which data would be acquired continuously during injection along a set of fixed raypaths (Figure 1). Conceptually, if the CO₂ saturation and/or plume thickness increased along a given raypath, the travel time would decrease, thereby allowing detection with some spatial resolution, especially in the vertical direction. Obtaining continuous crosswell seismic data required deploying the seismic source and sensors via production tubing concurrently with a

geochemical fluid sampling system. The seismic source needed to be deployed on the outside of production tubing, within a small annular space. To address this limitation, we designed a novel "piezotube" source (Daley et al., patent pending). The source could then be deployed in the injection well for the duration of the injection.

ACCOMPLISHMENTS

Continuous crosswell seismic monitoring of a small-scale CO₂ injection was accomplished with the development of a novel tubing-deployed piezoelectric borehole source. This "piezotube" source, deployed on the CO₂ injection tubing near the top of the saline aquifer reservoir at 1,657 m depth, enabled acquisition of crosswell recordings at 15-minute intervals during the multiday injection. The change in travel time recorded at various depths in a nearby observation well allowed hour-by-hour monitoring of the growing CO₂ plume via the induced seismic velocity change (Figure 1).

SIGNIFICANCE OF FINDINGS

Our field-scale application of the CASSM methodology, along with the development of a tubing deployable source, demonstrates a novel approach for characterizing reservoir processes *in situ*. The travel-time measurements indicate that the CO₂ plume reached the top of the reservoir sand before reaching the observation well, thus providing information about the *in situ* buoyancy of CO₂. Potential applications include perimeter detection of migrating CO₂ and detailed crosswell "movies" of reservoir fluid movement.

RELATED PUBLICATIONS

- Daley, T.M., R.D. Solbau, J.B. Ajo-Franklin, and S.M. Benson, Continuous active-source monitoring of CO₂ injection in a brine aquifer. *Geophysics*, 71(5), 33-41, 2007.
Daley, T.M., L.R. Myer, J.E. Peterson, E.L. Majer, and G.M. Hoversten, Time-lapse crosswell seismic and VSP monitoring of injected CO₂ in a brine aquifer. *Environmental Geology* (in press), 2007.

ACKNOWLEDGMENTS

This work was conducted as part of the Geologic Carbon Sequestration (GeoSeq) Project, supported by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, through the National Energy Technology Laboratory, U.S. Department of Energy, under Contract No. DE-AC02-05CH11231.

MODELING GEOLOGIC STORAGE OF CARBON DIOXIDE: COMPARISON OF NONHYSTERETIC AND HYSTERETIC CHARACTERISTIC CURVES

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RESEARCH OBJECTIVES

Geologic storage of carbon dioxide (CO_2) in brine-bearing formations has been proposed as a means of reducing the atmospheric load of greenhouse gases. In the subsurface, supercritical CO_2 forms an immiscible gas-like phase and partially dissolves in the brine. Numerical models of CO_2 /brine systems use characteristic curves to represent the interactions of nonwetting-phase supercritical CO_2 and wetting-phase brine. The simplest characteristic curves are nonhysteretic—the capillary pressure and relative permeabilities depend only on the local saturation at the current time. A more sophisticated approach is a hysteretic formulation, in which capillary pressure and relative permeabilities depend not only on the current value of the local saturation, but on the history of the local saturation and the process that is occurring: drainage (replacement of wetting phase with nonwetting phase) or wetting (replacement of nonwetting phase with wetting phase, also known as imbibition). The objective of this research is to investigate the impact of using nonhysteretic or hysteretic characteristic curves to model various aspects of CO_2 geological storage.

APPROACH

Two example problems involving geologic CO_2 storage are simulated with TOUGH2, a multiphase, multicomponent code developed at Berkeley Lab for flow and transport through geologic media. TOUGH2 considers all flow and transport processes relevant for a two-phase (liquid-gas), three-component (CO_2 , water, dissolved NaCl) system. Both a nonhysteretic and a newly developed hysteretic formulation are employed to represent characteristic curves, to illustrate the applicability and limitations of nonhysteretic methods. The first application considers leakage of CO_2 from the storage formation to the ground surface, while the second examines the role of heterogeneity within the storage formation.

ACCOMPLISHMENTS

Simulation results show drastically different behavior for the long-term evolution of CO_2 plumes for nonhysteretic and hysteretic formulations. For an idealized problem that involves only drainage or only wetting, a

nonhysteretic formulation, in which capillary pressure and relative permeability depend only on the current value of the grid-block saturation, would be adequate. However, for a more realistic problem that includes both injection of CO_2 (a drainage

process) and its subsequent postinjection evolution (a combination of drainage and wetting), hysteretic characteristic curves are required to correctly capture the behavior of the CO_2 plume. This finding is a consequence of the fact that residual gas saturation S_{gr} (the saturation below which free-phase CO_2 is trapped) is strongly process-dependent, with a zero value during drainage and a potentially large value during imbibition, a value that increases with the maximum local historical value of gas saturation.

SIGNIFICANCE OF FINDINGS

During post-injection periods, the leading edge of the CO_2 plume undergoes drainage ($S_{gr}=0$), while the trailing edge undergoes wetting (large S_{gr}). Thus, the plume is more mobile at the leading edge and less mobile at the trailing edge, so it elongates. In addition to trapping significant quantities of free-phase CO_2 at the trailing edge of the plume, this elongation enables more CO_2 to dissolve in the brine and greater interaction with rock minerals to occur, further immobilizing CO_2 . It is impossible to correctly model these processes using a nonhysteretic formulation for characteristic curves.

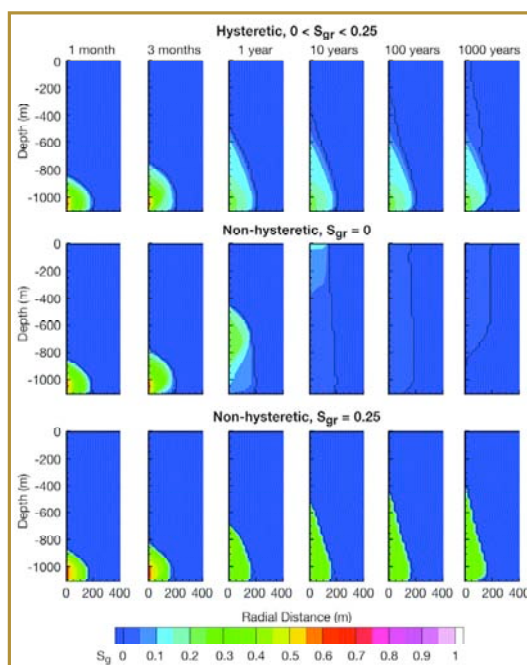


Figure 1. Free-phase CO_2 distributions at a series of times for hysteretic (top) and nonhysteretic (middle and bottom) formulations for characteristic curves. CO_2 injection at 1,000 m depth lasts for one month. Neither nonhysteretic case can model the post-injection period in which the CO_2 plume is more mobile at the top than at the bottom and a small amount of CO_2 reaches the surface while the bulk of the plume remains trapped at depth.

RELATED PUBLICATION

Doughty, C., Modeling geologic storage of carbon dioxide: comparison of non-hysteretic and hysteretic characteristic curves. *Energy Conversion and Management* 48(6), 1768–1781, 2007.

Related web site: <http://www-esd.lbl.gov/GEOSEQ/index.html>

ACKNOWLEDGMENTS

This work was conducted as part of the Geologic Carbon Sequestration (GeoSeq) and Zero Emissions Research and Technology (ZERT) projects, supported by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, through the National Energy Technology Laboratory, U.S. Department of Energy, under Contract No. DE-AC02-05CH11231.

SITE CHARACTERIZATION FOR CO₂ GEOLOGIC STORAGE AND VICE-VERSA—THE FRIO BRINE PILOT, TEXAS, AS A CASE STUDY

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RESEARCH OBJECTIVES

Geologic storage of carbon dioxide (CO₂) in brine-bearing formations has been proposed as a means of reducing the atmospheric load of greenhouse gases. Careful site characterization is critical for successful geologic storage of CO₂, because of the many physical and chemical processes impacting CO₂ movement and containment in the subsurface. Traditional site characterization techniques—such as geological mapping, geophysical imaging, and well logging and testing—provide the basis for judging whether or not a site is suitable for CO₂ storage. However, only through the injection and monitoring of CO₂ itself can the coupling between buoyancy flow, geologic heterogeneity, and history-dependent multiphase flow effects be observed and quantified. The purpose of this work is to demonstrate that CO₂ injection and monitoring can provide a valuable addition to the site-characterization process.

APPROACH

At the Frio brine pilot, a research project located in Dayton, Texas, 1,600 metric tons of CO₂ were injected over a period of 10 days into a steeply dipping brine-saturated sand layer at a depth of 1,500 m. The pilot is used as a case study to illustrate an iterative sequence in which traditional site characterization is used to prepare for CO₂ injection, and then monitoring of the CO₂ injection itself is used to further site-characterization efforts.

Numerical modeling plays a central role in integrating geological, geophysical, and hydrological field observations. In the subsurface, supercritical CO₂ forms an immiscible gas-like phase that is strongly buoyant and partially dissolves in the brine. The numerical simulator TOUGH2 considers all flow processes relevant for a two-phase (liquid-gas), three-component (CO₂, water, dissolved NaCl) system, including newly developed hysteretic formulations for capillary pressure and relative permeability functions.

ACCOMPLISHMENTS

Pre-injection activities included traditional site-characterization techniques, such as review of the regional geology, development of a local geological model, analysis of wireline logs, laboratory analysis of core samples, chemical analysis of brine samples, pressure-transient analysis of an interference well test, and breakthrough curve analysis for a two-well recirculation tracer test. Additionally, the CO₂ injection itself served as an interference well test by monitoring downhole pressure in both wells and as a two-well tracer test by sampling fluid at the observation well using a novel U-tube configuration. Geophysical monitoring of CO₂ movement in the subsurface during and after the injection period provided information on the spatial distribution of CO₂ at different scales. CO₂-saturation-sensitive well logs were run periodically in both injection and observation wells,

crosswell seismic was conducted in the plane between the injection and observation wells before and after CO₂ injection, and vertical seismic profiles (VSP) monitored the CO₂ plume as it migrated beyond the immediate vicinity of the wells.

By comparing field observations to model results, we obtained both an improved understanding of the local geology and better-constrained values of multiphase flow parameters (see Figure 1).

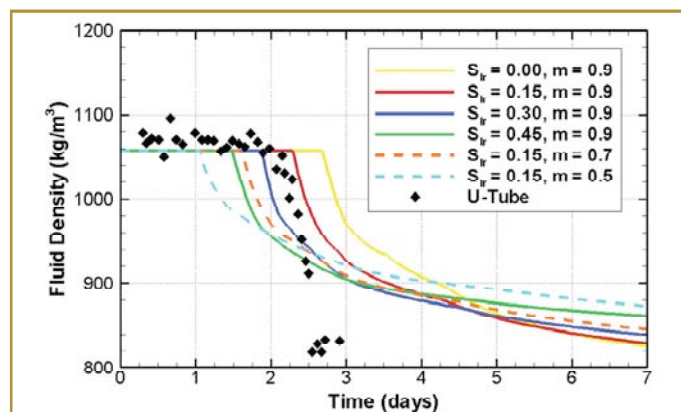


Figure 1. CO₂ arrival at observation well as monitored with U-tube sampling and model results for the 8 m sand model considering different two-phase flow parameters: S_{Lr} is residual liquid saturation, and m quantifies the interference between liquid and gas phases.

SIGNIFICANCE OF FINDINGS

Well thought-out site characterization is essential for successful geologic storage of CO₂, and the site-characterization process greatly benefits from the addition of CO₂ injection and monitoring.

RELATED PUBLICATION

Doughty, C., B.M. Freifeld, and R.C. Trautz, Site characterization for CO₂ geologic storage and vice versa—The Frio brine pilot, Texas, USA, as a case study. Environmental Geology DOI 10.1007/s00254-007-0942-0, 2007.

ACKNOWLEDGMENTS

This work was conducted as part of the Geologic Carbon Sequestration (GeoSeq) Project, supported by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, through the National Energy Technology Laboratory, U.S. Department of Energy, under Contract No. DE-AC02-05CH11231.

RELATED WEB SITE

<http://www-esd.lbl.gov/GEOSEQ/index.html>



EDDY COVARIANCE MEASUREMENTS OF CO₂ EMISSIONS AT MAMMOTH MOUNTAIN, CALIFORNIA

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RESEARCH OBJECTIVES

The eddy covariance (EC) method, a micrometeorological technique traditionally used to measure CO₂ fluxes across the interface between the atmosphere and a plant canopy, has been proposed as a viable technique to monitor for CO₂ leakage from geologic storage sites. EC provides the benefit of an automated flux measurement that is averaged over both time and space. However, the theory that underlies EC assumes spatial homogeneity of surface fluxes and flat terrain, conditions that are not typically met at sites being considered for CO₂ storage. The objective of this work is to evaluate the quality of EC CO₂ flux measurements made at Mammoth Mountain, California, a site that challenges the basic assumptions of EC with complex terrain and high, spatially heterogeneous CO₂ emission rates.

APPROACH

An EC station was deployed on Mammoth Mountain from September 8, 2006, to October 24, 2006. EC CO₂ fluxes were calculated by time averaging over half-hour periods the product of the time series of fluctuating vertical wind velocity and atmospheric CO₂ concentration, measured at a fixed height above the ground surface. Surface CO₂ fluxes were also measured at point locations on a grid using the chamber method, repeatedly over a ten-day period. EC fluxes were compared to chamber fluxes through the footprint model, a weighting function that describes the relative contribution of each point source surface flux to the EC flux. On any given day, the grid of chamber CO₂ flux measurements was weighted by the half-hour EC footprint function (hereafter referred to as the footprint CO₂ flux) and compared to the half-hour EC flux.

ACCOMPLISHMENTS

The mean and standard deviation of the relative difference between the EC and footprint CO₂ fluxes, expressed as a percentage of the footprint flux, were -0.3 and 23%, respectively, indicating that the measurements were nearly unbiased. A plot of EC versus footprint CO₂ flux (Figure 1a) shows that the data are moderately correlated ($R^2 = 0.42$ for 1:1 line). The correlation increases ($R^2 = 0.70$ for 1:1 line) for average daily EC versus average daily footprint CO₂ flux (Figure 1b).

SIGNIFICANCE OF FINDINGS

EC CO₂ fluxes were measured at a site that challenged the underlying assumptions of EC theory. Variability in the EC and footprint flux datasets was likely caused by our inability to completely characterize spatial-temporal variations in surface CO₂ fluxes using the chamber method, as well as by inherent random errors associated with both the EC and chamber methods.

Average daily EC and footprint CO₂ fluxes were well correlated, indicating that when random error is reduced by temporal averaging,

the EC technique can perform well under certain challenging site conditions. EC has the potential to be reliably used for leakage monitoring at CO₂ storage sites.

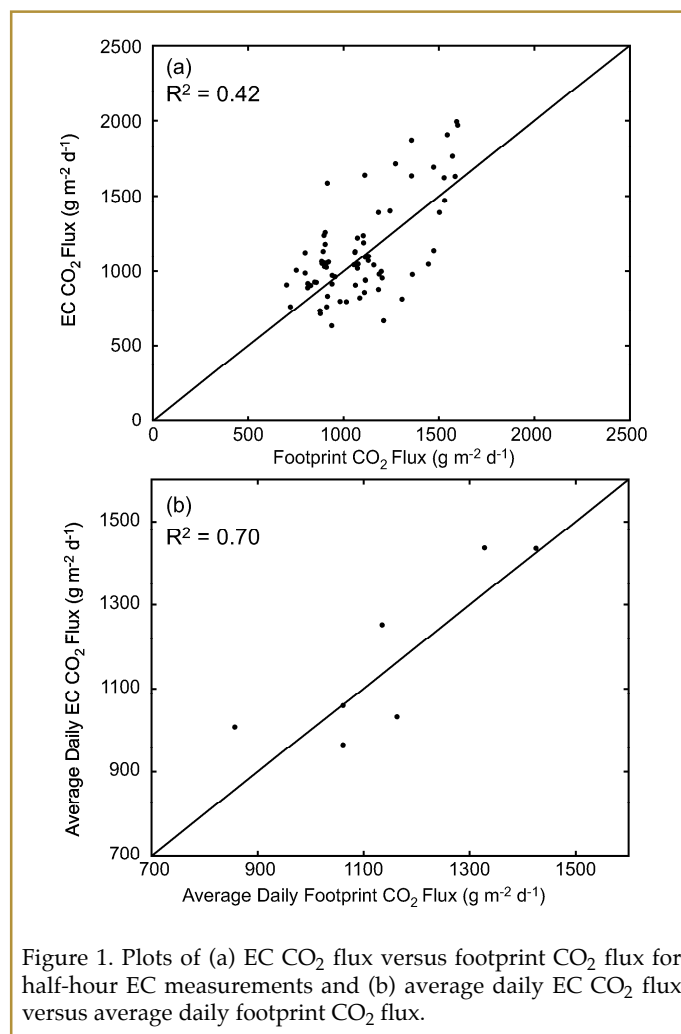


Figure 1. Plots of (a) EC CO₂ flux versus footprint CO₂ flux for half-hour EC measurements and (b) average daily EC CO₂ flux versus average daily footprint CO₂ flux.

RELATED PUBLICATION

Lewicki, J.L., G.E. Hilley, T. Tosha, R. Aoyagi, K. Yamamoto, and S.M. Benson, Dynamic coupling of volcanic CO₂ flow and wind at the Horseshoe Lake tree kill, Mammoth Mountain, California. *Geophysical Research Letters*, 34, L03401, doi:10.1029/2006GL028848, 2007.

ACKNOWLEDGEMENTS

This work was supported by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, through the National Energy Technology Laboratory, U.S. Department of Energy under Contract No. DE-AC02-05CH11231.



NATURAL ANALOGUES FOR CO₂ LEAKAGE FROM GEOLOGIC STORAGE SITES

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RESEARCH OBJECTIVES

While the purpose of geologic carbon storage is to trap CO₂ underground, CO₂ could migrate away from the storage site into the shallow subsurface and atmosphere. Although limited CO₂ leakage does not negate the net reduction of CO₂ emissions to the atmosphere, adverse health, safety, and environmental risks associated with elevated CO₂ concentrations must be evaluated. Cases of CO₂ leakage from natural reservoirs to the near-surface environment serve as analogues for the potential release of CO₂ from geologic storage sites. The objective of this research is to summarize and compare the features, events, and processes (FEPs) of CO₂ leakage examples from natural geologic reservoirs. We describe causes and consequences of CO₂ leakage, and discuss implications for geologic carbon storage and risk assessment work.

APPROACH

Carbon dioxide leakage cases were classified according to (1) key features of the CO₂ accumulation, including site location, the source of the CO₂, and the geologic model for CO₂ accumulation; (2) the events leading to leakage from the reservoir; and (3) the processes by which CO₂ was released at the surface, including the pathway(s) for leakage and the style of surface emission. Cases from volcanic, geothermal, and sedimentary basin settings were considered.

ACCOMPLISHMENTS

Key FEPs were identified for a wide range of CO₂ leakage cases. Here, we show one example from each major geologic setting (Table 1).

SIGNIFICANCE OF FINDINGS

Four general FEPs were identified based on analysis of a range of natural analogues for CO₂ leakage, from which lessons can be learned and should be applied to risk assessment associated with geologic carbon storage:

- (1) CO₂ can both accumulate beneath, and be released from, primary and secondary reservoirs with capping units located at a wide range of depths. Both primary and secondary reservoir entrapments for CO₂ should be properly characterized at potential geologic carbon sequestration sites.
- (2) Many CO₂ releases have been correlated with a specific event that has triggered the release, such as magmatic or seismic activity. The potential for processes that could cause

geomechanical damage to sealing cap rocks and trigger the release of CO₂ from a storage reservoir should be evaluated.

- (3) Unsealed fault and fracture zones can act as fast and direct conduits for CO₂ flow from depth to the surface. Risk assessment should therefore emphasize determining the potential for and nature of CO₂ migration along these structures.
- (4) The style of CO₂ release at the surface varies widely between and within different leakage sites. In rare circumstances, the release of CO₂ can be a self-enhancing and/or eruptive process; this possibility should be assessed in the case of CO₂ leakage from storage reservoirs.

Table 1. Examples of FEPs of natural leakage of CO₂

Site	CO ₂ Source	Geologic model for accumulation	Event triggering leakage	Pathway for leakage	Type of surface leakage
Mammoth Mountain, CA USA	Magmatic + thermal decomposition of carbonates	Accumulation at ~2 km depth in porous/fracture d rock under caprock	Seismic activity and reservoir pressurization	Faults and fractures	Fast, diffuse, vent, spring
Latera caldera, Italy	Thermal decomposition of carbonates, magmatic component	CO ₂ accumulates in liquid-dominated, carbonate geothermal reservoir capped by hydrothermally altered volcanics	No specific leakage event captured	Faults and fractures	Diffuse, vent, spring
Paradox Basin, UT, USA	Thermal decomposition of carbonates	Reservoirs are vertically stacked, sandstone units, in fault-bounded anticlinal folds, capped by shale/siltstone units	No specific leakage event captured	Faults and fractures	Diffuse, gas seeps, springs

RELATED PUBLICATION

Lewicki, J.L., J. Birkholzer, and C.-F. Tsang, Natural and industrial analogues for leakage of CO₂ from storage reservoirs: Identification of features, events, and processes and lessons learned. *Environmental Geology*, doi:10.1007/s00254-006-0479-7, 52, 2007.

ACKNOWLEDGEMENTS

This work was supported by the U.S. Environmental Protection Agency, Office of Water and Office of Air and Radiation, under an Interagency Agreement with the U.S. Department of Energy at the Lawrence Berkeley National Laboratory, Contract No. DE-AC02-05CH11231.



CERTIFICATION FRAMEWORK (CF) FOR GEOLOGIC CO₂ STORAGE

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RESEARCH OBJECTIVES

Critical to the large-scale deployment of carbon dioxide capture and storage (CCS) is a simple, transparent, and accepted basis for regulators and stakeholders to certify that the risks of geologic CCS projects to health, safety, and the environment (HSE) are acceptable. The objective of this effort is to develop a simple, transparent, and accepted framework for evaluating leakage risk for certifying operation and decommissioning of geologic CO₂ storage sites.

APPROACH

The U.S. EPA's Underground Injection Control (UIC) program is used successfully to regulate deep injection of liquids. Under the most stringent set of regulations, injected liquid is required not to migrate away from the injection zone for 10,000 years. This is the so-called non-migration requirement. There are fundamental differences between liquids regulated under the UIC program and geologic CO₂ storage, differences that make a nonmigration requirement inappropriate for CCS. For example, vastly larger volumes of CO₂ will be injected relative to hazardous liquid-waste disposal, and the buoyancy of supercritical CO₂ creates an upward driving force for migration. Under the conditions applicable to CO₂ storage, we propose an effective trapping requirement analogous to the non-migration requirement of the UIC program. In the CF, effective trapping, based on CO₂ leakage risk (CLR), is the overarching requirement for safety and effectiveness of a CO₂ storage site. With user input on subsurface properties, wells, faults, vulnerable assets, and injection parameters, the CF calculates the CLR for a given site. In the CF, CO₂ leakage risk is defined as the product of impact and probability of impact ($CLR = I \times P$). Impacts are assumed to occur when CO₂ enters one or more of the following compartments at a rate above an agreed-upon limit:

ECA = Emission Credits and Atmosphere

HSE = Health, Safety, and Environment

USDW = Underground Sources of Drinking Water

HMR = Hydrocarbon and Mineral Resources

Reservoir simulation is used to calculate CO₂ fluxes with time into compartments. Fluxes and concentrations are either read from a catalog of pre-simulated results or computed on a site-specific basis. Probabilities of the injected CO₂ plume intersecting wells and/or faults (P_{wf}), and of wells and/or faults intersecting compartments (P_{ic}), are based on input data on well and fault density, along with computed CO₂ plume geometry. CF is probabilistic in existence of a flow pathway and

deterministic in flow along the pathway. If the CLR is below threshold values, then the CO₂ is considered effectively trapped, meaning that the storage site is safe and effective. A flow chart of the CF approach is presented in Figure 1.

ACCOMPLISHMENTS

We have developed a framework for calculating CO₂ leakage risk to various compartments. We have assembled a ten-member international advisory board from whom we get feedback and comments on our approach. We are currently carrying out a case study using the framework to evaluate a hypothetical CO₂ storage project in the Texas Gulf Coast.

SIGNIFICANCE OF FINDINGS

The CF is a simple and transparent framework in which limited leakage is allowable, as long as the leakage risk is below agreed-upon thresholds.

RELATED PUBLICATIONS

Oldenburg, C.M., and S.L. Bryant, Certification framework for geologic CO₂ storage. LBNL-63395 Abs. Sixth Annual Conference on Carbon Capture and Sequestration, Pittsburgh, PA, May 8–10, 2007

ACKNOWLEDGMENT

This work was supported in part by the CO₂ Capture Project (CCP) of the Joint Industry Program (JIP), and by Lawrence Berkeley National Laboratory under Department of Energy Contract No. DE-AC02-05CH11231.

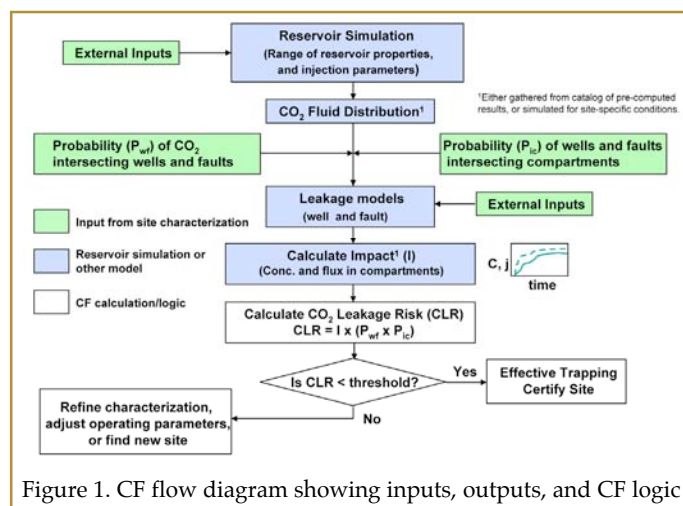


Figure 1. CF flow diagram showing inputs, outputs, and CF logic

SIMULATIONS OF CO₂ RELEASE FOR THE ZERT MONTANA SHALLOW RELEASE EXPERIMENT

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RESEARCH OBJECTIVES

Demonstrations by the technical community of the ability to detect, characterize, mitigate, and remediate CO₂ seepage from geologic CO₂ storage sites are needed to satisfy public concerns about the safety and environmental impact of geologic CO₂ storage. To develop and demonstrate approaches for detection and characterization of CO₂ seepage, the Zero Emissions Research Technology (ZERT) team constructed a shallow CO₂ release facility in an agricultural field on the Montana State University (MSU) campus. The idea behind the facility is to emulate CO₂ seepage through direct injection of CO₂ at shallow depths. The facility consists of a 70 m long horizontal well approximately 2.5 m deep. The well is packed off into six sections, into which CO₂ is injected independently to model leakage through a linear feature such as a fault or fracture. In the study presented here, numerical simulations of CO₂ release are carried out to provide modeling support for experiment design and data interpretation.

APPROACH

The simulator TOUGH2/EOS7CA (Oldenburg and Unger, 2003; 2004) is used to model CO₂ injections into the shallow subsurface at the MSU site for two sets of experiments: (1) shallow vertical-well injection using a 2-D radial grid; and (2) shallow horizontal-well injection using a 2-D cartesian grid. The shallow subsurface at the MSU site consists of 1.2 m of soil overlying a cobble formation, with water table at approximately 1.5 m depth. The shallow vertical-well injection consisted of a 1.6 L/min (4.8×10^{-5} kg/s) CO₂ injection at a depth of approximately 3 m. Seepage fluxes were measured in the field using an accumulation chamber around the injection well in the N, S, E, and W directions. Measured CO₂ seepage fluxes were used as constraints to fit appropriate model permeabilities to the soil and cobble layers. Subsequently, these fitted soil and cobble properties were used in forward models for design and prediction of the horizontal release experiment.

ACCOMPLISHMENTS

Presented in Figure 1 (top) is the simulated vertical-injection well seepage flux (solid lines) along with the measured data showing the fit obtained for $k_{\text{soil}} = 5 \times 10^{-11}$ m² (50 D), and $k_{\text{cobble}} = 3.2 \times 10^{-12}$ m² (3.2 D). The high inferred permeability of the soil likely arises from cracks and root casts that create macropores through which soil gas and atmospheric air readily flow. Figure 1 (bottom) shows simulated results for the horizontal well. Various injection rates were simulated. The 100 kg/d rate predicted breakthrough after 1.5 days and seepage fluxes that were neither too easy nor too difficult to detect ($q_{\text{max}} \sim 100$ $\mu\text{moles}/(\text{m}^2 \text{ s})$ (380 g/(m² d)). The subsequent field experiment, run at an injection rate of 100 kg/d, resulted in the collection of field data using a variety of approaches that generally agreed with the predictive calculations.

SIGNIFICANCE OF FINDINGS

That shallow soils can be very permeable to upward CO₂ seepage is a key finding of this research project. The implication is that CO₂ in the shallow subsurface can easily migrate upwards and seep out of the ground, where various monitoring approaches may be used for characterizing the seepage.

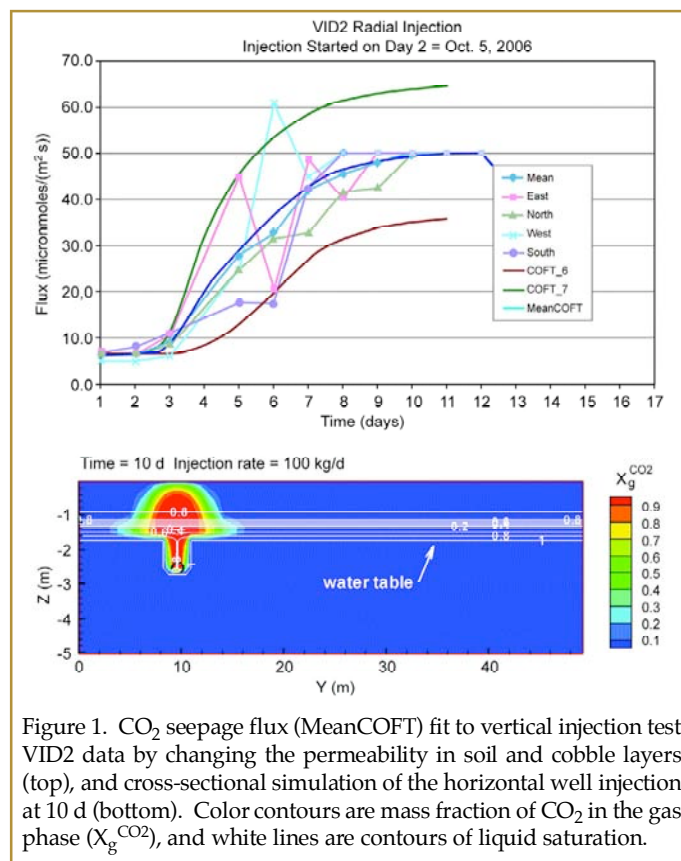


Figure 1. CO₂ seepage flux (MeanCOFT) fit to vertical injection test VID2 data by changing the permeability in soil and cobble layers (top), and cross-sectional simulation of the horizontal well injection at 10 d (bottom). Color contours are mass fraction of CO₂ in the gas phase ($X_g^{\text{CO}_2}$), and white lines are contours of liquid saturation.

RELATED PUBLICATIONS

- Oldenburg, C.M., and A.J.A. Unger, On leakage and seepage from geologic carbon sequestration sites: Unsaturated zone attenuation. LBNL-51928. Vadose Zone Journal, 2(3), 287–296, August 2003. .
- Oldenburg, C.M., and A.J.A. Unger, Coupled vadose zone and atmospheric surface-layer transport of CO₂ from geologic carbon sequestration sites. LBNL-55510. Vadose Zone Journal, 3, 848–857, 2004.

ACKNOWLEDGMENTS

This work was conducted as part of the Zero Emissions Research and Technology (ZERT) Project, supported by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, through the National Energy Technology Laboratory, U.S. Department of Energy, under Contract No. DE-AC02-05CH11231.



JOULE-THOMSON COOLING DUE TO CO₂ INJECTION INTO NATURAL GAS RESERVOIRS

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RESEARCH OBJECTIVES

Depleted natural gas reservoirs are a promising target for the storage of anthropogenic CO₂ as a greenhouse gas mitigation strategy. One effect of injecting CO₂ into a low-pressure (depleted) gas reservoir is Joule-Thomson cooling. Potential problems that could arise from Joule-Thomson cooling include the formation of CO₂ and/or CH₄ hydrates, freezing of residual water and associated reduction in injectivity, and generation of thermal stresses that could fracture the formation. The purpose of this study is to use numerical simulation to investigate the magnitude of Joule-Thomson cooling that may arise during CO₂ injection into depleted CH₄ reservoirs.

APPROACH

We used a simple one-dimensional radial geometry to represent an idealized depleted gas reservoir (Figure 1, top). Production is idealized as being from the outermost gridblock at a distance of 1100 m in a five-spot pattern. We used the TOUGH2 module called EOS7C (Oldenburg et al., 2004), which models five components (water, brine, noncondensable gas, tracer, and methane) under isothermal or nonisothermal conditions. The subroutines used in EOS7C are available as a web-based tool to calculate properties of gas mixtures (<http://esdtools.lbl.gov/gaseos/home.html>). We verified the methods used in EOS7C for expansion-related cooling by modeling the classical Joule-Thomson experiment, in which gas flows at constant enthalpy from a bulb at high pressure to a bulb at lower pressure as the temperature change is recorded. Simulated results agreed well with reference values.

ACCOMPLISHMENTS

Here we present a single example simulation consisting of a constant-rate CO₂ injection at 3 kg/s with an injection temperature and initial reservoir temperature of 45°C (Figure 1, bottom). Production of CH₄ occurs at a rate of 0.56 kg/s. Shown in Figure 1 are results for $k = 10^{-14}$ m² (10 mD). As shown, cooling is approximately 8°C over a 100 m radius from the well after 15 years of injection, not enough to cause any concerns for hydrates, freezing, or thermal stresses. The simulation study

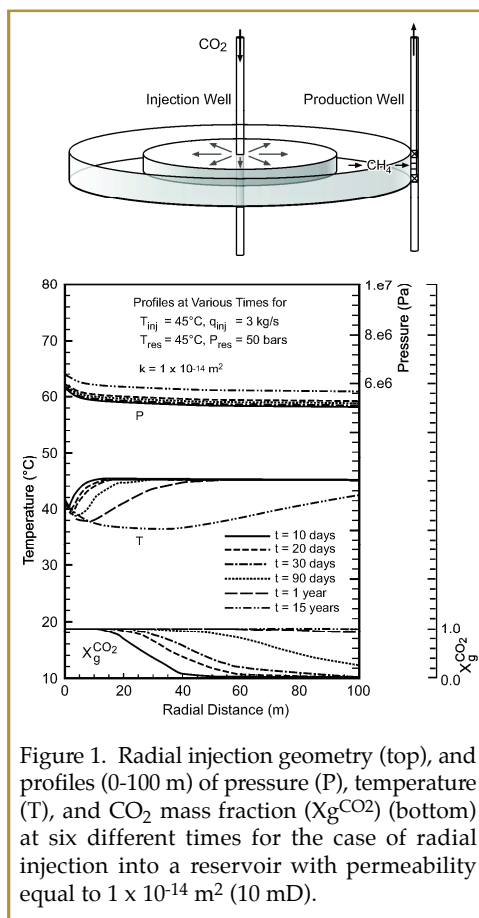


Figure 1. Radial injection geometry (top), and profiles (0-100 m) of pressure (P), temperature (T), and CO₂ mass fraction (X_g^{CO₂}) (bottom) at six different times for the case of radial injection into a reservoir with permeability equal to 1×10^{-14} m² (10 mD).

showed that for a constant injection rate, lower permeability causes larger ΔP and correspondingly larger ΔT , owing to Joule-Thomson cooling. We also confirmed that low-porosity allows more heat to be provided by the matrix grains to offset Joule-Thomson cooling. Therefore, the effects of permeability and porosity may partially compensate, although it appears the effect of permeability is larger than the effect of porosity.

SIGNIFICANCE OF FINDINGS

Joule-Thomson cooling during constant-rate CO₂ injection is larger for lower permeability reservoirs and higher porosity reservoirs. The simulation results show that Joule-Thomson cooling is a minor effect (<4°C) for low-injection rates and for permeabilities in the range expected in the Sacramento Valley. Overall, the conclusion from this study is that Joule-Thomson cooling is not expected to be a significant obstacle to successful CO₂ storage in depleted or depleting gas reservoirs.

RELATED PUBLICATIONS

- Oldenburg, C.M., Joule-Thomson cooling due to CO₂ injection into natural gas reservoirs. LBNL-60158. Energy Conversion and Management, 48, 1808-1815, 2007.
- Oldenburg, C.M., G.J. Moridis, N. Spycher, and K. Pruess, EOS7C Version 1.0: TOUGH2 module for carbon dioxide or nitrogen in natural gas (methane) reservoirs. LBNL-56589, March 2004.

ACKNOWLEDGMENT

This work was conducted as part of the West Coast Regional Carbon Sequestration Partnership (WESTCARB) (specifically, the Sacramento Valley applications) and Zero Emissions Research and Technology (ZERT) (specifically, code development) projects, supported by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, through the National Energy Technology Laboratory, U.S. Department of Energy, under Contract No. DE-AC02-05CH11231.

ECO2N: A TOUGH2 FLUID PROPERTY MODULE FOR MIXTURES OF WATER, NaCl, AND CO₂

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RESEARCH OBJECTIVES

Numerical simulation plays a key role in evaluating the feasibility of storing CO₂ in geologic formations—identifying favorable as well as unfavorable hydrogeologic conditions at proposed storage sites, designing and analyzing tests, and optimizing storage design. The purpose of this work was to develop accurate and robust simulation capabilities, and to make such capabilities available to the technical community.

APPROACH

The desired simulation capability was developed as an enhancement of our existing multipurpose reservoir simulation code TOUGH2. Building on a fluid property module EWASG for mixtures of saline brine and CO₂, and on previously developed research codes for CO₂ storage, a new module ECO2N was developed as an add-on to TOUGH2.

ACCOMPLISHMENTS

The new ECO2N module includes a comprehensive description of the thermodynamics and thermophysical properties of H₂O-NaCl-CO₂ mixtures, one that reproduces fluid properties largely within experimental error for the temperature, pressure, and salinity conditions of interest (10°C ≤ T ≤ 110°C; P ≤ 600 bar; salinity up to full halite saturation). Flow processes can be modeled isothermally or nonisothermally, and phase conditions represented may include a single (aqueous or CO₂-rich) phase, as well as two-phase mixtures. Fluid phases may appear or disappear in the course of a simulation, and solid salt may precipitate or dissolve. ECO2N uses newly developed correlations that accurately predict the partitioning of water and CO₂ between immiscible brine and CO₂-rich phases. A detailed user's guide was written that gives technical specifications of ECO2N, includes instructions for preparing input data, and provides illustrative applications to several sample problems, including problems that had been previously investigated in a code intercomparison study.

As an example, Figure 1 presents an application of TOUGH2/ECO2N to a simplified version of the first industrial-scale CO₂ aquifer storage project in the Norwegian sector of the North Sea.

SIGNIFICANCE OF FINDINGS

The ECO2N module was released to the public through DOE's Energy Science and Technology Software Center (ESTSC). It is available to licensees of TOUGH2 at no additional charge, and has been quickly adopted by many groups in academia and industry, both nationally and internationally.

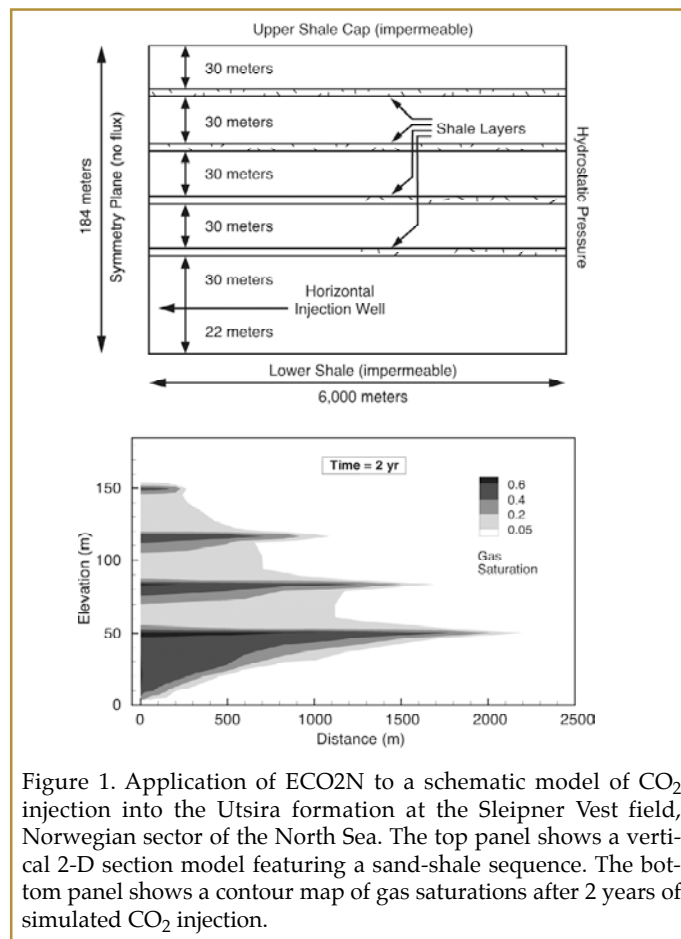


Figure 1. Application of ECO2N to a schematic model of CO₂ injection into the Utsira formation at the Sleipner Vest field, Norwegian sector of the North Sea. The top panel shows a vertical 2-D section model featuring a sand-shale sequence. The bottom panel shows a contour map of gas saturations after 2 years of simulated CO₂ injection.

RELATED PUBLICATIONS

- Pruess, K., ECO2N: A TOUGH2 fluid property module for mixtures of water, NaCl, and CO₂. LBNL-57592, Berkeley, CA, June 2005.
- Pruess K., and N. Spycher. ECO2N—A fluid property module for the TOUGH2 code for studies of CO₂ storage in saline aquifers. *Energy Conversion and Management*, 48(6), pp. 1761–1767, doi:10.1016/j.enconman.2007.01.016, 2007.

ACKNOWLEDGMENTS

This work was conducted as part of the Zero Emissions Research and Technology (ZERT) Project, supported by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, through the National Energy Technology Laboratory, U.S. Department of Energy, under Contract No. DE-AC02-05CH11231.



ANALYSIS OF FAULT RUPTURE AND CO₂ UPWELLING DURING THE 1960s MATSUSHIRO EARTHQUAKE SWARM AS A NATURAL ANALOGUE OF CO₂ STORAGE AND LEAKAGE

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RESEARCH OBJECTIVES

This study is part of a collaborative research between Berkeley Lab and Japanese organizations on the Matsushiro Earthquake Swarm that occurred in central Japan in the mid-1960s. During the five-year term of the swarm, between 1965 to 1970, approximately 60,000 earthquakes were felt, and ten million tons of CO₂-bearing water appeared at the ground surface, flowing up through newly created surface ruptures. One part of this research project, described herein, was to use coupled reservoir-geomechanical modeling to understand the effects of a deep high-pressure CO₂ source on the initiation and propagation of the fault ruptures that resulted in the Matsushiro Earthquake Swarm.

APPROACH

The coupled CO₂ fluid flow and geomechanical processes, including fault motion and associated permeability changes, were modeled using the TOUGH-FLAC coupled reservoir-geomechanical simulator. A model for fault permeability changes with fault reactivation was implemented into the TOUGH-FLAC simulator. Then a series of two and three-dimensional simulations were conducted to identify key parameters and investigate possible causes and mechanisms behind the Matsushiro Earthquake Swarm.

ACCOMPLISHMENTS

Figure 1 shows a three-dimensional model domain and the results of fault-rupture distribution associated with the upwelling CO₂. The geomechanical analysis explains the cause of the Matsushiro Earthquake Swarm as overpressure caused by the upwelling CO₂ fluid. The mechanisms of the earthquake are attributed to shear failure initiated by reduced effective stress on pre-existing fracture planes within and near the two main faults. It is concluded that the *in situ* three-dimensional stress regime, as well as fault strength and permeability, are likely the most important parameters that control the nucleation, propagation, arrest and occurrence of the earthquake swarm during its two years of migration through the seismogenic crust. Moreover, surface deformation and increased seismicity were found to be precursors to the CO₂ surface release, because these mechanical responses were detected up to a year before any chemical changes were measured at the ground surface.

SIGNIFICANCE OF FINDINGS

The analysis of the Matsushiro Earthquake Swarm is an example of how natural analogues can provide a greater understanding of the factors controlling retention and leakage of CO₂. Specifically, it was demonstrated that geomechanical modeling tools and monitoring approaches

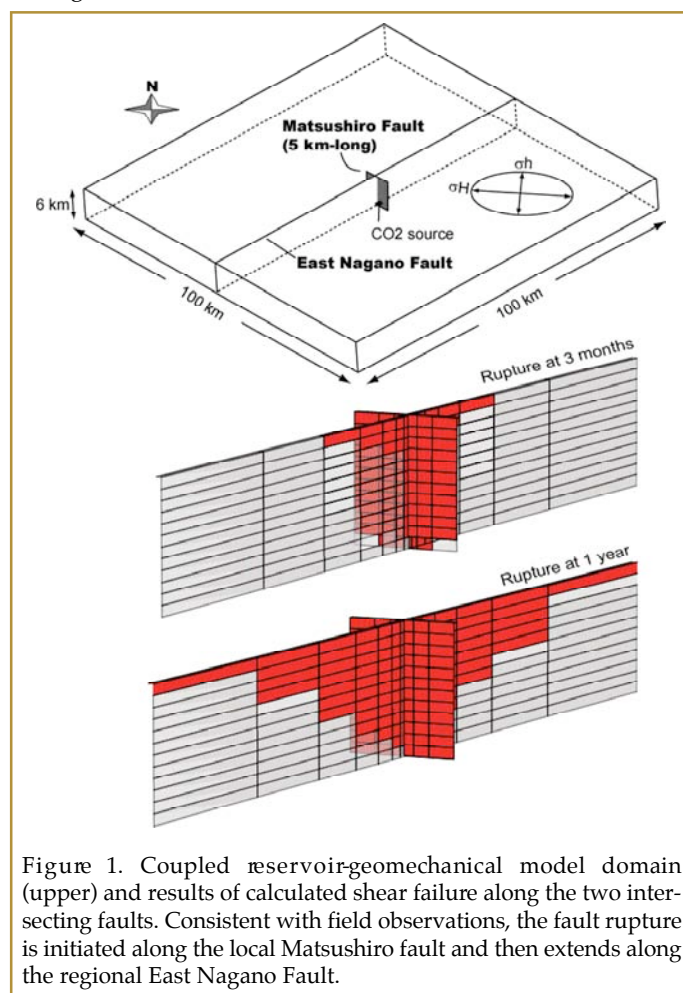
available today can help improve our understanding and quantifying of the factors leading to leakage of CO₂. Such an understanding will be needed to avoid selecting sites where the probability of leakage is high, and to quantify leakage should it occur.

RELATED PUBLICATION

Yamamoto, K., R. Aoyagi, H. Koide, T. Tosha, S. Nakanishi, N. Todaka, S. Benson, J. Rutqvist, and J. Lewicki, Matsushiro earthquake swarm (1965–1967) as natural analogue of CO₂ storage and leakage. *Eos Trans. AGU*, 87(52), Fall Meeting, Suppl., Abstract H21A-1359, (2006).

ACKNOWLEDGMENTS

The work presented in this paper was financed by the Ministry of Economy, Trade, and Industry (METI) of Japan through the Mizuho Information and Research Institute.



COUPLED RESERVOIR-GEOMECHANICAL ANALYSIS OF GEOMECHANICAL DAMAGE ASSOCIATED WITH CO₂ GEOLOGIC STORAGE

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RESEARCH OBJECTIVES

The objective of this research is to study factors affecting the maximum sustainable injection pressure and the potential for mechanical failure associated with deep underground injection of carbon dioxide (CO₂). Large-scale underground injection of CO₂ may involve a substantial increase in reservoir pressure, which will induce mechanical stresses and deformations in and around the injection reservoir. If reservoir pressure becomes too large in the overlying caprock formations, new fractures or faults may be created there or existing ones reactivated. This could provide flow paths for CO₂ to escape, thereby substantially reducing the effectiveness of sequestration.

APPROACH

Using the TOUGH-FLAC coupled reservoir-geomechanical simulator, we conducted a study of hydromechanical processes during injection of supercritical CO₂ into deep brine formations. We investigated the possibility of rock-mechanical failure in the form of hydraulic fracturing or shear slip reactivation of existing faults.

ACCOMPLISHMENTS

We have analyzed mechanical stress changes and the potential for mechanical failure associated with underground injection of CO₂. Figure 1 shows an example of simulation results for CO₂ injection into an injection zone overlain by several aquifers and caprock units. In this case, a vertical fault zone allowed for limited upward migration of the CO₂ through the two first caprock layers, affecting the potential for shear failure in overlying units. One important conclusion from this study is that the potential for mechanical failure, and the type and orientation of failure, depends to a large extent on the initial stress field (stress regime). As such, the stress field should be much more carefully measured and monitored than is typical in the current practice for oil and gas explorations. Furthermore, the potential for mechanical failure should be analyzed for the entire region affected by mechanical stress changes, which is generally more extensive than the region of fluid pressure change at depth.

SIGNIFICANCE OF FINDINGS

Results from this study may be important input when developing possible guidelines for site investigations and for estimating

maximum sustainable injection pressure at a geological CO₂ injection site. For example, potential mechanical failure at shallow levels above the injection zone may need to be assessed.

RELATED PUBLICATIONS

Rutqvist J., J. Birkholzer, F. Cappa, and C.F. Tsang, Estimating maximum sustainable injection pressure during geological sequestration of CO₂ using coupled fluid flow and geomechanical fault-slip analysis. *Energy Conversion and Management* 48(6), 1798–1807, 2007.

Rutqvist, J., J.T. Birkholzer, and C.F. Tsang, Coupled reservoir-geomechanical analysis of the potential for tensile and shear failure associated with CO₂ injection in multilayered reservoir-caprock systems. *Int. J. Rock Mech. & Min. Sci.*, 45(1), 132-142, 2007.

ACKNOWLEDGMENTS

This work was conducted with funding from the U.S. Environmental Protection Agency, Office of Water and Office of Air and Radiation, under an Interagency Agreement with the U.S. Department of Energy at the Lawrence Berkeley National Laboratory, and with funding from the Assistant Secretary for Fossil Energy, Office of Coal and Power Systems, through the National Energy Technologies Laboratory, under Department of Energy Contract No. DE-AC02-05CH11231.

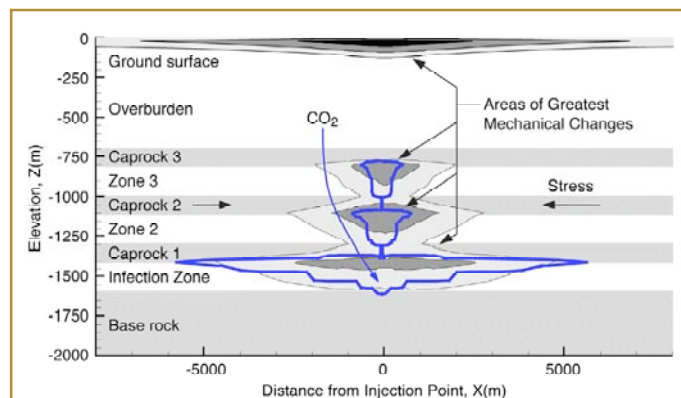


Figure 1. Migration of CO₂ (blue contour line) and potential for shear failure (gray scale contours) after 30 years of injection into an injection zone overlain by multiple caprock layers. In this case, the stress regime is compressional, i.e., the horizontal stress is higher than the vertical.

A MODEL OF BUOYANCY-DRIVEN EVOLUTION OF A CARBON DIOXIDE PLUME

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RESEARCH OBJECTIVES

This work is motivated by the growing interest in injecting carbon dioxide into deep geologic formations as a means of avoiding its atmospheric emissions and consequent contribution to global warming. One of the key questions regarding the feasibility of this technology is the potential rate of leakage out of the primary storage formation. Here, we perform a model-based study and theoretical prediction of evolution of a gas plume in an aquifer flowing upward under buoyancy.

APPROACH

We seek simple analytical solutions in a model of two-phase flow of supercritical gas and brine. We focus on the role of interactions among buoyancy, viscous, and capillary forces. To achieve this objective, we assume homogeneous formation and neglect the heat and chemical transport and phase change processes. We consider vertical countercurrent flow, which takes place in the central part of a laterally spread plume or in a permeable fault.

ACCOMPLISHMENTS

Our principal finding is that the evolution of the saturation profile of a moving plume can be described as a sequence of traveling and rarefaction waves. Driven by buoyancy, the plume propagates by stretching vertically upward, unlike a gas bubble in water. It has been established that the Darcy velocity of each fluid reaches its maximum near the top of the original plume location. This maximum-flow point is characterized by a constant fluid saturation and does not move during evolution of the plume. The fluid displacement mechanism above this location is drainage, whereas below it, it is imbibition. The velocity of plume propagation and the fluid saturation in the leading part of the plume have been expressed through the properties of the formation and the fluids. The calculations suggest that the velocity of propagation for a plume of supercritical carbon dioxide can be on the order of tens of meters per year in an aquifer whose permeability is on the order of 100 millidarcies (Figure 1).

SIGNIFICANCE OF FINDINGS

Characterization of plume propagation is crucially important for development of optimal injection technologies to maximize greenhouse gas trapping and sequestration. Possible leakage of injected carbon dioxide to the surface could result in

health and safety concerns. Development of monitoring policies in the areas near gas storage sites will benefit from theoretical estimates of plume propagation velocity.

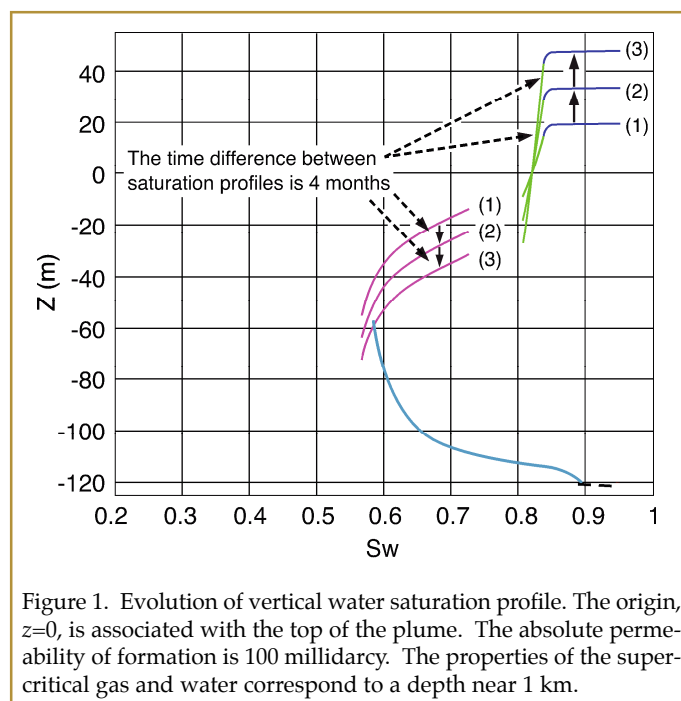
RELATED PUBLICATIONS

Silin, D., T.W. Patzek, and S.M. Benson, Exact solutions in a model of vertical gas migration. SPE paper 103156. In: 2006 SPE Annual Technical Conference and Exhibition, SPE, San Antonio, TX, September 24–27, 2006.

Silin, D., T.W. Patzek, and S.M. Benson, A model of buoyancy-driven two-phase countercurrent fluid flow. LBNL-62607. Transport in Porous Media (in press), 2007.

ACKNOWLEDGMENTS

This work was conducted as part of the Zero Emissions Research and Technology (ZERT) Project, supported by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, through the National Energy Technology Laboratory, U.S. Department of Energy, under Contract No. DE-AC02-05CH11231.



DEVELOPMENT OF AN EFFICIENT PARALLEL SIMULATOR FOR MODELING CO₂ GEOLOGIC SEQUESTRATION IN SALINE AQUIFERS

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RESEARCH OBJECTIVES

Carbon dioxide geologic sequestration in saline aquifers involves very complex multiphase flow processes. Numerical modeling can play an important role in evaluating the feasibility and reliability of CO₂ disposal. However, modeling of these processes in general requires fine spatial and temporal discretization, and also may require coverage of a large simulation domain, all of which represent a large computational challenge. The objective of this study is to develop an efficient parallel simulator for these types of simulations.

APPROACH

The parallel simulation approach is based on the ECO2N module of the TOUGH2 code. The parallel simulator retains all the process-modeling capabilities of the original TOUGH2/ECO2N and parallel computation features of TOUGH2-MP. In this study, a domain decomposition approach is adopted for model parallelization and MPI (message passing interface) for parallel implementation. The code partitions the simulation domain, defined by an unstructured grid, using a partitioning algorithm from the METIS software package. In a parallel simulation, each processor handles one portion of the simulation domain for updating thermophysical properties, assembling mass and energy-balance equations, solving linear equation systems, and performing other local computations. Local linear-equation systems are solved in parallel by multiple processors with the Aztec linear solver package. The parallel simulator has been built with efficient communication schemes.

ACCOMPLISHMENTS

An efficient parallel simulator for large-scale, long-term CO₂ geologic sequestration in saline aquifers has been developed. The parallel simulator is a three-dimensional, fully implicit model that solves large, sparse linear systems arising from discretization of the mass- and energy- balance equations in porous and fractured media. The simulator provides a comprehensive description of the thermodynamics and thermophysical properties of H₂O-NaCl-CO₂ mixtures, and models single and/or two-phase isothermal or nonisothermal flow processes, two-phase mixtures, appearance or disappearance of fluid phases, and salt precipitation or dissolution.

The code demonstrates excellent scalability. Test runs show that a linear or super-linear speedup can be obtained on Linux clusters as well as on supercomputers (See Figure 1). Because the parallel simulator was developed from an existing mature code, it inherits not only simulation functions from the original

code, but also all other features, including input/output format, error handling, and improvements for code stability. These features provide robustness for the parallel code and ease of use for the user community of the original code.

SIGNIFICANCE OF FINDINGS

The domain decomposition approach and parallel computation enhance model simulation capabilities, in terms of problem size and complexity, to a level that cannot be reached by single-CPU codes. By using the parallel simulator, multimillion grid-block problems can be run on a typical Linux cluster with several tens to hundreds of processors to achieve a ten to hundred times improvement in computational time or problem manageability.

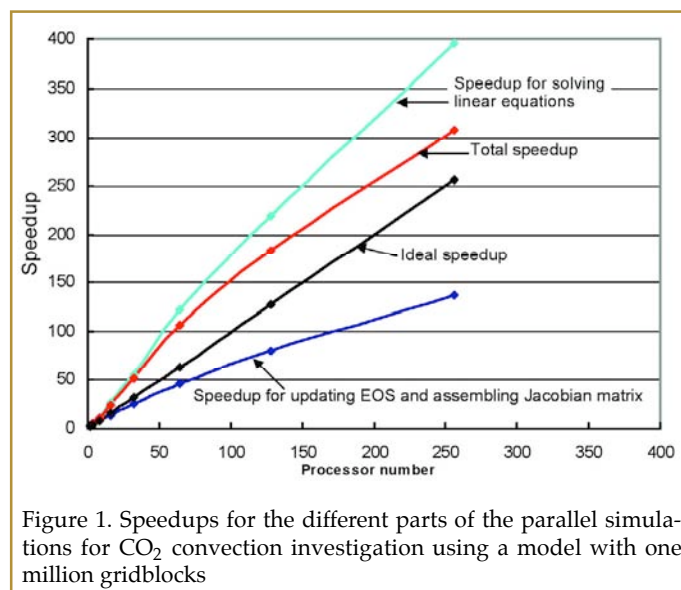


Figure 1. Speedups for the different parts of the parallel simulations for CO₂ convection investigation using a model with one million gridblocks

RELATED PUBLICATION

Zhang, K., C. Doughty, Y-S Wu, and K. Pruess, Efficient parallel simulation of CO₂ geologic sequestration in saline aquifers. Paper SPE 106026, Proceedings of the 2007 SPE Reservoir Simulation Symposium, Houston, Texas, 2007.

ACKNOWLEDGMENTS

This work was conducted as part of the Zero Emissions Research and Technology (ZERT) project, supported by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, through the National Energy Technology Laboratory, U.S. Department of Energy, under Contract No. DE-AC02-05CH11231.



SYSTEM-LEVEL MODELING FOR ECONOMIC EVALUATION OF GEOLOGIC CO₂ STORAGE IN GAS RESERVOIRS

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RESEARCH OBJECTIVES

The objective of this study is to develop a system-level model that has the capability to evaluate the economic and environmental impacts of geological CO₂ storage under uncertainty. This system model specifically evaluates the feasibility of carbon sequestration with enhanced gas recovery (CSEGR) in the Rio Vista region of California. Implemented within this model are CO₂ capture and separation, compression, pipeline transportation to the storage site, and CO₂ injection into and methane out of a gas reservoir. The subsurface component of the system is calculated based on simulations from a detailed process model of the gas reservoir.

APPROACH

A top-down method is used to build a hierarchical model for the studied CSEGR system. First, CSEGR subsystems are identified and connected to track CO₂ and CH₄ flows (Figure 1). Next, components of each subsystem are identified and connected. Finally, potential features, events and processes (FEPs) are identified, and corresponding feedbacks are incorporated within the system. The level of detail increases at lower levels of the system hierarchy. The advantage of this top-down method (over a bottom-up method) is that processes in different sectors can be properly coupled and their feedbacks properly considered.

The system-level analysis is performed using GoldSim (www.goldsim.com), a flexible probabilistic simulation platform. The reservoir simulations are performed using EOS7C (Oldenburg et al., 2004), a TOUGH2 module for multicomponent gas mixtures.

ACCOMPLISHMENTS

We have developed a system-level model for analyzing geological storage of CO₂. Our system model includes detailed reservoir simulations of CO₂ injection, CH₄ displacement and production, and potential leakage through a fault or abandoned well. The associated environmental consequences are evaluated. Using process simulation embedded in a system-level model, the economic benefits of CO₂ sequestration and enhanced gas recovery can be directly weighed against the costs of CO₂ injection.

SIGNIFICANCE OF FINDINGS

There is much research effort being conducted to improve understanding of factors affecting particular aspects of geological CO₂ storage (such as storage performance, storage capacity, and health, safety, and environmental [HSE] impacts), as well as to lower the cost of CO₂ capture and related processes. However, there has been less emphasis to date on system-level analyses of

geologic CO₂ storage that consider geologic, economic, and environmental issues by linking detailed process models to representations of engineering components and associated economic models. This study provides a framework/capability for feasibility evaluations on geological CO₂ storage under uncertainty, and can be extended to other waste management operations.

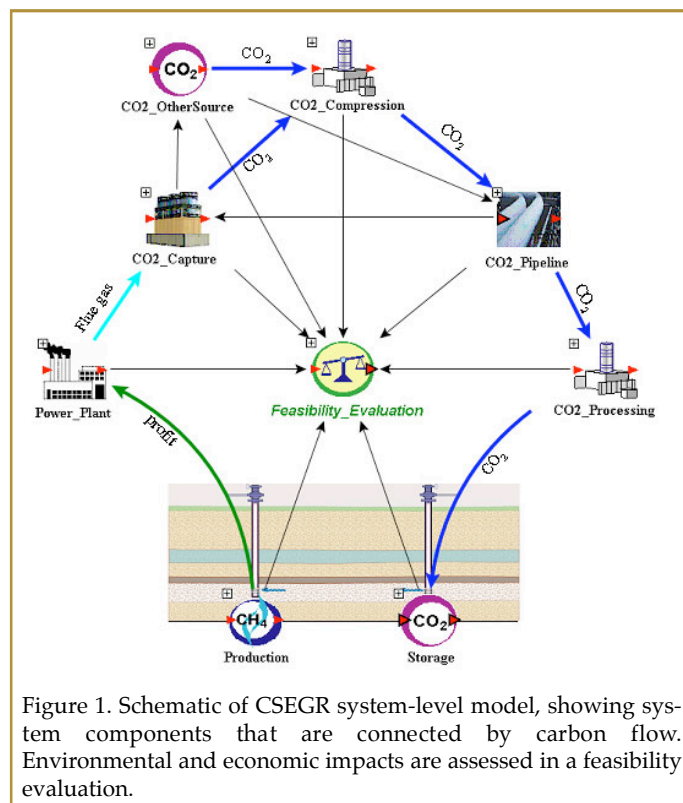


Figure 1. Schematic of CSEGR system-level model, showing system components that are connected by carbon flow. Environmental and economic impacts are assessed in a feasibility evaluation.

RELATED PUBLICATION

Zhang, Y., C.M. Oldenburg, S. Finsterle, and G.S. Bodvarsson, System-level modeling for economic evaluation of geological CO₂ storage in gas reservoirs. *Energy Conservation and Management*, 48, 1827-1833, doi:10.1016/j.enconman.2007.01.018, 2007.

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